Journal of Physical Chemistry B 2012 vol.116 N39, pages 11959-11967

Steady-state homogeneous nucleation and growth of water droplets: Extended numerical treatment

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Abstract

The steady-state homogeneous vapor-to-liquid nucleation and the succeeding liquid droplet growth process are studied for water systems by means of the coarse-grained molecular dynamics simulations with the mW model suggested originally by Molinero et al. [Molinero, V.; Moore, E. B. J. Phys. Chem. B2009, 113, 4008-4016]. The investigation covers the temperature range $273 < T/K < 363$ and the systems pressure $p \simeq 1$ atm. The thermodynamic integration scheme and the extended mean first passage time method as tools to find the nucleation and cluster growth characteristics are applied. The surface tension is numerically estimated and is compared with the experimental data for the considered temperature range. We extract the nucleation characteristics such as the steady-state nucleation rate, the critical cluster size, the nucleation barrier, and the Zeldovich factor and perform the comparison with the other simulation results and test the treatment of the simulation results within the classical nucleation theory. We found that the liquid droplet growth is unsteady and follows the power law. Also, the growth laws exhibit the features unified for all of the considered temperatures. The geometry of the nucleated droplets is also studied. © 2012 American Chemical Society.

http://dx.doi.org/10.1021/jp304830e